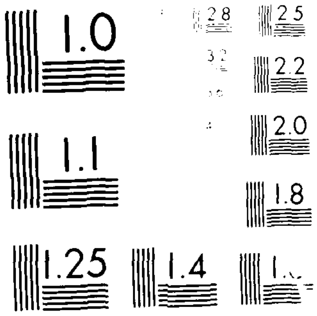
AD-A191 469 THE CHARACTERIZATION OF SOLUTES AND SOLVENT PHASES(U) 1/1
SURREY UNIV GUILDFORD (ENGLAND) M H ABRAHAM ET AL.
14 OCT 87 DAJA45-87-C-0004

UNCLASSIFIED F/G 7/4 NL

END
DATE
FILMED
5 88
DTIC


1.0
2.8
2.5
2.2
2.0
1.1
1.8
1.25
1.4

AD-A191 469

(2)

THE CHARACTERIZATION OF SOLUTES & SOLVENT PHASES

PROGRESS REPORT **14 OCTOBER 1987**

Dr Michael H. Abraham

Mr Gary S. Whiting

University of Surrey, Guildford, Surrey, U.K.

Contract No. DAJA45-87-C-0004

R&D 5390-CH-01

88 2 11 019

Summary

The characterisation of five gas-liquid chromatographic stationary phases, using retention data obtained by Laffort and co-workers for 240 solutes, has been carried out by the method of multiple linear regression analysis. Relative gas-liquid partition coefficients for as many solutes as possible were correlated against various combinations of parameters. The best general equation was found to be one containing the exploratory variables π_2^*, δ, α_m, β_m, and $\log L^{16}$. Attempts to replace π_2^* by the dipole moment (μ^2) were not very successful, and neither were attempts to use refractive index functions or molar refractions in combination with μ^2. However, replacement of π_2^* by the dipole moment itself was more successful, and led to quite good equations in μ, δ, α_m, β_m, and $\log L^{16}$.

A number of new $\log L^{16}$ values have been determined experimentally, using the gas-chromatographic method.

Introduction

Over the past few years, Abraham, Doherty, Kamlet, Taft and co-workers[1,2] have constructed equations for the correlation and prediction of a very large number of physicochemical and biochemical phenomena. These equations are based on a cavity theory of solution, in which the process of dissolution of a solute in a solvent may be broken down into a number of hypothetical steps: (i) the endoergic formation of a cavity in the bulk solvent, (ii) rearrangement of solvent molecules round the cavity, and (iii) the exoergic interaction of the solute with the surrounding solvent molecules after the solute has been inserted into the cavity. If the Gibbs energy change in step (ii) is zero, or very nearly zero as is usually assumed, only steps (i) and (iii) need to be modelled. The energy of formation of a cavity can be taken as proportional to the solvent cohesive energy density, $(\delta_H^2)_1$, where δ_H is the Hildebrand solubility parameter, and to some function of the solute size, or volume, V_2,⁺ leading to a term $(\delta_H^2)_1.V_2$ with the units of energy. Various solvent-solute interactions can take place in step (iii). If both solvent and solute are dipolar, a term in $\pi_1^*.\pi_2^*$ will arise, where π^* is the solvent or solute dipolarity. Hydrogen-bond interactions will also be set up, either between a solvent acting as a hydrogen-bond base and a solute acting as a hydrogen-bond acid, $\beta_1.\alpha_2$, or between a solvent acting as the acid and the solute as the base, $\alpha_1.\beta_2$. In these two terms, α_1 and β_1 refer to the solvent hydrogen-bond acidity and basicity, and α_2 and β_2 to the solute hydrogen-bond acidity and basicity. The full equation for the correlation of some solubility related property, SP, is then given by the multiple linear regression equation,

---

⁺ We denote, as usual, solvent properties by the subscript 1 and solute properties by the subscript 2.

$$SP = A + B\pi_1^{*}\pi_2^{*} + C\beta_1\alpha_2 + D\alpha_1\beta_2 + E(\delta_H^2)_1 V_2 \qquad (1)$$

Now for a process involving a series of solutes in a given solvent, all the solvent parameters in equation (1) are constant, leading to equation (2). For solutes that are aromatic or polyhalogenated, a polarisability

$$SP = C + s.\pi_2^{*} + a.\alpha_2 + b.\beta_2 + M.V_2 \qquad (2)$$

correction term is needed, which takes the form $\delta_2 = 1$ for aromatic solutes, 0.5 for polyhalogenated solutes, and zero for all other solutes. This leads to the final equation, used extensively in the correlation of a wide variety of phenomena in condensed phases, equation (3). An early application of

$$SP = C + s.\pi_2^{*} + d.\delta_2 + a.\alpha_1 + b.\beta_2 + m.V_2 \qquad (3)$$

equation (3) to a process involving a gaseous phase, namely the solubility of gases and vapours in polymers,[3] revealed a possible deficiency in that equation (3) contains no term that corresponds to solute-solvent dispersion, or van der Waals, interaction. An alternative equation was therefore put forward, with a new solute parameter, log L^{16}, replacing the volume term V_2. This new parameter was defined as the logarithm of the solute Ostwald solubility coefficient, L, on n-hexadecane at 298K.[4]

$$L = \frac{\text{concentration of solute in solution}}{\text{concentration of solute in the gas phase}} \qquad (4)$$

Two possible equations for the correlation of the solubility of a series of gases and vapours in a given condensed phase are therefore equations (3) and (5), and we set out to investigate the use of these two equations. There are several ways of describing the solubility of gases in liquids, but in view

of the use of the Ostwald solubility coefficient in equation (5) shall define gas solubility through equation (4). It should be noted that L is actually the same as the gas-liquid partition coefficient, K, used in the description of gas-liquid chromatography (GLC). The coefficient L or K is related to the specific retention volume at the column temperature, V_G, through equation (6) where ρ_1 is the stationary phase density.

$$SP = C + s.\pi_2^* + d.\delta_2 + a.\alpha_2 + b.\beta_2 + 1.\log L^{16} \qquad (5)$$

$$L \text{ (or K)} = \beta_1 . V_G \qquad (6)$$

In order to apply equations (3) and (5), values of SP (i.e. log L or Log V_G) should be available for a wide selection of solutes on the same liquid phase. By far the most convenient and accurate method of obtaining such a series of SP values is by GLC itself, and there are numerous compilations of such data. Probably the most extensive, carefully measured, values are those recorded by Laffort and co-workers[5] for 240 solutes on 5 stationary phases, and this is the data we have chosen first to analyse. Laffort and co-workers published their data in the form of Kovat's retention indices, defined for isothermal GLC through equation (7).

$$I(x) = 100 \frac{\log V_G(x) - \log V_G(Pn)}{\log V_G(Pn + 1) - \log V_G(Pn)} + 100n \qquad (7)$$

Here, I(x) is the retention index of solute x, V_G is the specific retention volume, and (Pn) and (Pn + 1) represent n-alkanes of carbon number n and N + 1. The equation used to calculate their retention indices is,

$$I = 100 \frac{\log \tau(x) - \log \tau(P_{10})}{b} + 1000 \qquad (8)$$

where $\tau(x)$ and $\tau(P_{10})$ are the corrected retention times for compound x and n-decane, and b is the slope for n-alkanes. From equation (6) and equation (8) it follows that

$$\log L(x) = \frac{I-1000}{100} b + \log L(P_{10}) \tag{9}$$

and hence values of log L(x) may be calculated for the 240 solutes relative to log L for n-decane. These relative values of $\log L(x) - \log L(P_{10})$ can be used in equations (3) and (5) to yield exactly the same coefficients etc. as would be found with the absolute values of log L(x).+ The constant quantity $\log L(P_{10})$ will be subsumed into the value of C.

The five phases studied by Laffort and co-workers are listed in Table 1, and the 240 solutes are given in Table 2. In Table 3 are given those listed in our database, i.e. those for which we had some, or most, of the required solute parameters and in Table 4 are the b-values used in equation (9). The parameters that were chosen to be used in regressions are as follows:

π_2^* These values are those that have been extensively used by Kamlet and co-workers.[1,2,7-10]

δ_2 This is a trivially-calculated parameter, taken as 1.0 for aromatic solutes, 0.5 for polyhalogenated solutes, and zero for all others.

$\alpha_2(\alpha_m)$ These values were taken from recent papers of Kamlet and co-workers.[7-10]

+ This is not the case if only Kovat's retention indices are known. It is therefore fortunate that Laffort and co-workers[5] had the foresight to record values of b for each of the five stationary phases studied. Note that slightly different b-values are given in Laffort's table III. We are indebted to Professor Laffort[6] for suggesting that those in the first two would be the most suitable to use in our equation (9).

$\alpha_2(\alpha_2^H)$ This is a new hydrogen-bond acidity parameter recently developed by Abraham and co-workers using log K values for hydrogen-bond complexation.[11]

$\beta_2(\beta_m)$ These were, again, taken from papers of Kamlet and co-workers.[7-10]

$\beta_2(\beta_2^H)$ This is a new hydrogen-bond basicity parameter,[12] obtained by the same procedure as α_2^H.

$V_2(V_x)$ In all our calculations we used the trivially calculatable characteristic volume, as detailed by Abraham and McGowan.[13]

log L^{16} Many of values were taken from the experimental paper of Abraham, Grellier, and McGill.[4] Other values have been obtained in this work, see experimental section and the section on log L^{16} values.

μ_2 Dipole moments were taken from standard literature sources.[14,15]

$f(n^2)$ This refractive index function, defined as $f(n^2) = (n^2-1)/(n^2+2)$ was calculated from literature values of the refractive index of the solute liquid at 293 K and the sodium-D line.[16]

MR The molar refraction was obtained from the usual definition, MR $= f(n^2).M/P$, where M and P are the solute molecular weight and density; MR is the same as the electron polarisation, P_E.

MR_x To eliminate the need for a new parameter (the density), a modified molar refraction was calculated as $MR_x = f(n^2).V_x$.

In the present report, we set out equations, based on the α_m and β_m values of Kamlet and co-workers,[7-10] and in a subsequent report we shall investigate the use of the new parameters α_2^H and β_2^H. To some extent equations (3) and (5) are straightforward in that, apart from α_m and β_m taken as standard, the other parameters V_x and log L^{16} are well-defined solute parameters. However π_2^* is partly derived from the solvent parameter π_1^*, and

partly obtained through a dipole moment correlation. One aim of the present work was therefore to see if π_2^* could be replaced either by the dipole moment (μ or μ^2) or some combination of dipole moment with $f(n^2)$ or MR. Of course, another aim is to obtain the best regression equation that could be used to predict new values of the chromatographic parameter.

Results and discussion

Regressions were run for the relative values of log L(x) on the five phases listed in Table 1. The coefficients of the parameters are listed in a series of Tables, together with the number of data points (n), the multiple correlation constant (r), and the standard deviation (s.d.). Also given are the per cent confidence levels for the coefficients (correlation %). The Tables are as follows:

Table 5:	δ, π_2^*, α_m, β_m, Vx	All phases
	$f(n^2)$, μ^2, α_m, β_m, Vx	
Table 6:	δ, π_2^*, α_m, β_m, log L^{16}	All phases
	$f(n^2)$, μ^2, α_m, β_m, log L^{16}	
Table 7:	δ, μ^2, α_m, β_m, Vx	Polyph ether only
	δ, μ^2, α_m, β_m log L^{16}	
	MR_x, μ^2, α_m, β_m, Vx	
	MR_x, μ^2, α_m, β_m, log L^{16}	

Since the various regressions in μ^2 were not very good, an additional series was run that included only solutes with a single dominant dipole moment - i.e. solutes such as acids, esters, nitro compounds and so forth were removed. Further regressions were carried out as follows:

Table 8:	$f(n^2)$, μ^2, α_m, β_m, Vx	TCEP only
	$f(n^2)$, μ^2, α_m, β_m, log L^{16}	
	MR_x, μ^2, α_m, β_m, VX	
	MR_x, μ^2, α_m, β_m, log L^{16}	

Although μ^2 is theoretically a better parameter to use than μ itself, two sets of regressions were run using μ as a dipolar parameter. In each set, regressions were carried out for all solutes for which parameters were available, and for solutes with $\delta = 0$:

Table 9:	$f(n^2)$, μ, αm, βm, log L^{16}	All phases
Table 10:	δ, μ, αm, βm, log L^{16}	All phases
	μ, αm, βm, log L^{16}	

A direct comparison of Tables 5 and 6 shows quite clearly that regressions in log L^{16} are always markedly superior to those in Vx, and hence we shall consider only the log L^{16} correlations henceforth. Results in Table 6 for the general equation (5) are quite good, with correlation constants ranging from 0.9943 to 0.9805 for the five phases with about 90 solutes. The constants in equation (5) make general chemical sense: all five phases are hydrogen-bond bases and have no hydrogen-bond acidity, and hence the coefficient in the term $b.\beta_m$ should be statistically not significant. This is true for all the phases except Zonyl E7. This phase is supposed to be a

fluorinated ester of "pyromellitic acid and a trihydrofluoro alcohol". The former is 1,2,4,5-benzene tetra-carboxylic acid, and it is possible that the commercial product contains either unesterified carboxylic acid or hydroxyl groups.

One difficulty over a physicochemical interpretation of equation (5) is that polarisability effects are contained in the $s.\pi_2^*$ term as well as on the $d.\delta$ term. It would be particularly useful if the dipolarity and polarisability effects, both contained in $s.\pi_2^*$, could be separately counted. To this end, we have investigated the effect of replacing the δ/π_2^* terms by various combinations of the dipole movement, as μ^2, and polarisability functions such as $f(n^2)$ or MR. In Table 6 are results of a direct replacement in equation (5) of π_2^* and δ by $f(n^2)$ and μ^2. The overall correlation constants are not as good as those in the original equation (5), but are not too bad. However, most surprisingly, the $b.\beta_m$ terms are statiscally significant for all five phases, thus making the entire regression equations rather suspect from a chemical point of view.

In Table 7 are results of replacing π_2^* and δ by either μ^2 and δ or by μ^2 and MR_x, for the polyphenyl ether phase as an example. There is an excellent correlation with δ, μ^2, α_m, β_m, and $\log L^{16}$ with $r = 0.9922$ and $sd = 0.093$, which must be close to an exhaustive fit. But once again, the $b.\beta_m$ term is highly significant. Regressions with $f(n^2)$ and μ^2 or MR_x and μ^2 for TCNE using a restricted set of solutes that contain either no dipole or else a single dominant dipole, are in Table 8. The only chemically reasonable regressions are those of the original form in δ/π_2^*.

Our conclusion as a result of the regressions set out in Tables 5-8 is that replacement of the δ/π_2^* symbolism by μ^2 in combination with a polarisability term leads (i) to regressions that are not as good, and (ii) to regressions that contain an unacceptable $b.\beta_m$ term.

In terms of chemical theory, correlations of an energy-related quantity such as log V_G or log L with dipole moment should certainly involve μ^2 and not μ. However, we thought it useful on an empirical level to investigate the use of μ as a solvent parameter. Table 9 gives details of regressions where $f(n^2)$ and μ replace δ and π_2^*. Once again, the $b.\beta_m$ term is highly significant for all five phases. Finally, in Table 10, are results of simply making a direct replacement of π_2^* by μ in equation(5), to give:

$$SP = C + s.\mu + d.\delta_2 + a.\alpha_2 + b.\beta_2 + l.\log L^{16} \qquad (10)$$

The regressions are all very good, and the only difficulty is that the $b.\beta_m$ term is still too significant for the phases TCEP, Polyphenyl ether, and DEGS. We carried out another set of regressions using equation (10) for a restricted set of solutes for which $\delta = 0$ (about 60-65 such solutes). The regression coeficients and sd values are the best we have obtained (compare Table 10 with Table 6), and now the $b.\beta_m$ terms are statistically not significant, as required (except for zonyl E7 !). We are much encouraged by the results in Table 10, and intend to pursue this line of regression analyses. If, indeed, π_2^* can be replaced by μ, not only would interpretation be much easier, but it would be possible to predict the dipole parameter rather easier from a knowledge of molecular structure.

Work in Progress

Further work is in hand on the refinement of equation (10) for the correlation and prediction of gas-liquid and gas-polymer partition coefficients. We hope that on the next report we shall be able to set out a modified equation (10) that will deal with the Laffort data set.

We also have in hand the analysis of a large number of log L values (or the equivalent log V_G values) on the nonpolar phases Apiezon and squalane. It

will be possible to extract from this data a rather extended list of secondary log L^{16} values that will considerably extend our data base.

Our next projected experimentation will be the acquisition of log L values for a range of solutes on some simple organic solvents, so that a direct comparison can be made with GLC stationary phases and with polymer phases.

Experimental

In order to increase the number of Laffort solutes for which we had all the parameters, additional log L^{16} values were determined, at the standard temperature of 298.15 K. A short column was used of length 50 cm and internal diameter 2 mm, containing 8.34% w/w of n-hexadecane on chromosorb B, mesh size 45/60. The standard used was n-octane of log L^{16} value 3.677, and Log L^{16} values for other solutes were obtained relative to n-octane, using a flame ionisation detector, as described before.[4] Results are given in Table 11. Attempts were also made to obtain log L^{16} values for proprionic acid and higher carboxylic acids, but without success, but further attempts will be made to determine these quantities, either directly or indirectly.

1. M. J. Kamlet, R. M. Doherty, J.-L. M. Abboud, M H. Abraham and R. W. Taft, Chemtech., 1986, 566.

2. M. H. Abraham, R. M. Doherty, M. J. Kamlet and R. W. Taft, Chem. Brit., 1986, 75, 629.

3. M. H. Abraham, P. L. Grellier, R. A. McGill, R. M. Doherty, M. J. Kamlet, T. N. Hall, R. W. Taft, P. W. Carr and W. J. Koros, Polymer, 1987, 28, 1363.

4. M. H. Abraham, P. L. Grellier and R. A. McGill, J.C.S. Perkin Trans. 2, 1987, 797.

5. F. Patte, M. Etcheto and P Laffort, Anal. Chem., 1982, 54, 2239.

6. Personal communication from Professor Laffort.

7. M. J. Kamlet, R. M. Doherty, G. D. Veith, R. W. Taft and M. H. Abraham, Envir. Sci. Tech., 1986, 20, 690.

8. M. J. Kamlet, R. M. Doherty, R. W. Taft, M. H. Abraham, G. D. Veith and D. J. Abraham, Envir. Sci. Tech., 1987, 21, 149.

9. M. J. Kamlet, R. M. Doherty, J.-L. M. Abboud, M. H. Abraham and R. W. Taft, J. Pharm. Sci., 1986, 75, 338.

10. M. J. Kamlet, R. M. Doherty, M. H. Abraham, P. W. Carr, R. F. Doherty and R. W. Taft, J. Phys. Chem., 1987, 91, 1996.

11. M. H. Abraham, P. P. Duce, P. L. Grellier, D. V. Prior, J. J. Morris and P. J. Taylor, in the press.

12. M. H. Abraham, P. L. Grellier, D. V. Prior, J. J. Morris, P. J. Taylor, C. Laurence and M. Berthelot, in the press.

13. M. H. Abraham and J. C. McGowan, Chromatographia, 1987, 23, 243.

14. A. L. McClellan, "Tables of Experimental Dipole Moments" pub. W. H. Freeman and Co.

15. R. J. W. le Fevre, Trans. Faraday Soc., 1934, Vol. 30, appendix.

16. Handbook of Chemistry and Physics.

Table 1. The five stationary phases studied by Laffort and co-workers.

Zonyl	Zonyl E7 (Dupont). This is a fluoro-ester.
CW 1540	Carbowax 1540 (Applied Science).
TCEP	Tricyanoethoxypropane
Polyph. ether	Polyphenyl ether, six rings.
DEGS	Diethyleneglycol succinate.

Table 2

Kovats retention indexes in GLC of 240 substances on five stationary phases. E corresponds to extrapolated values. The numbers of Handbook followed by * or an additional digit are not reported in the 50th edition but correspond to the same logic of classification.

Substances	Handbook	Zonyl	C.wax 1540	TCEP	Polyph. ether	DEGS
ALCOHOLS						
1 METHANOL	M0349	657	916	1228	522	1062
2 ETHANOL	E0334	704	933	1238	587	1083
3 1-PROPANOL	P1387	823	1045	1353	703	1188
4 ISOPROPANOL	P1388	741	916	1261	613	1057
5 ALLYL ALCOHOL	P1619	832	1112	1452	715	1284
6 1-BUTANOL	B2864	944	1164	1473	820	1311
7 ISOBUTANOL	P1633*	897	1104	1396	772	1242
8 2-BUTANOL	B2866	867	1023	1312	737	1149
9 TER-BUTANOL	P1633	816	949	1198	654	1036
10 1-PENTANOL	P0313	1055	1271	1502	924	1427
11 AMYL ALCOHOL(ACT C)	B2894	1010	1220	1514	884	1361
12 ISOAMYL ALCOHOL	B2895	1025	1229	1529	883	1375
13 TER-AMYL ALCOHOL	B2896	917	1014	1298	771	1162
14 CYCLOPENTANOL	C0092	1083	1337	1677	996	1518
15 1-HEXANOL	H0478	1160	1383	1691	1032	1644
16 2-HEXENOL(TRANS)	H0372*	1167	1416	1757	1044	1601
17 2-HEXANOL	H0480	1090	1241	1531	950	1384
18 3-HEXANOL	H0483	1065	1212	1497	941	1357
19 2-METHYL,2-PENTANOL	P0334	1022	1110	1393	848	1253
20 3-METHYL,3-PENTANOL	P0335	1038	1132	1427	909	1289
21 1-HEPTANOL	H0166	1262	1489	1794	1138	1648
22 2-HEPTENOL(TRANS)	H0209*	1278	1530	1880	1163	1737
23 1-OCTANOL	O0186	1370	1590	1902	1241	1764
24 2-OCTENOL(TRANS)	O0221*	1383	1639	1979	1262	1832
25 CIS,CIS,2,6-DIMETH CYCLOHEXANOL	C07511	1235	1423	1714	1168	1503
26 CIS,TR,2,6-DIMETH CYCLOHEXANOL	C07512	1297	1492	1826	1219	1687
27 TR,TR,2,6-DIMETH CYCLOHEXANOL	C07513	1272	1440	1737	1173	1614
28 2-METHYL,2-HEPTANOL	H0179	1222	1310	1582	1063	1433
29 3-METHYL,3-HEPTANOL	H0180	1220	1307	1584	1078	1456
30 1-NONANOL	N0543	1478	1712	2012	1350	1855
31 1-DECANOL	D0057	1371	1796	2102	1439	1959
32 A-TERPINEOL(DL)	T0049	1326	1709	2100	1426	1968
33 1-UNDECANOL	U0031	1702	1919	2234	1569	2088
34 1-DODECANOL	D0311	1813	2028	2343	1678	2208
35 EXO-ETHYL FENCHOL	F0013*	1360	1678	2010	1480	1890
ALDEHYDES						
36 ACETALDEHYDE	A0018	738	742	1073	541	914
37 PROPIONAL	P1083	830	825	1170	656	988
38 PROPENAL	P1707	842	864	1226	659	1053
39 BUTYRALDEHYDE	B2471	933	909	1263	753	1078
40 ISOBUTYRALDEHYDE	P1099*	887	834	1173	706	992
41 2-BUTENAL(TRANS)	B2933	1094	1086	1517	870	1305
42 ISOVALERALDEHYDE	B2481	1002	948	1290	813	1103
43 FURFURAL	F0277	1358	1495	2037	1135	1816
44 HEXANAL	H0316	1149	1113	1473	964	1294
45 2-HEXENAL(TRANS)	H0544	1313	1274	1712	1077	1502
46 HEPTANAL	H0090	1249	1224	1573	1066	1398
47 2-HEPTENAL(TRANS)	H0197*	1400	1363	1793	1172	1600
48 OCTANAL	O0110	1343	1311	1668	1167	1504
49 2-OCTENAL(TRANS)	O0208*	1287	1447	1729	1154	1602
50 BENZALDEHYDE	B0035	1452	1364	2076	1272	1845
51 SALICYLALDEHYDE	B0122	1521	1683	2194	1356	2030
KETONES						
52 ACETONE	P1649	904	839	1239	632	1034
53 2-BUTANONE	B2912	993	932	1329	764	1121
54 DIACETYL	B2632	1001	999	1498	772	1220
55 2-PENTANONE	P0344	1092	1030	1424	857	1230
56 CYCLOPENTANONE	C0094	1270	1258	1748	1050	1509
57 2-HEXANONE	H0317	1193	1123	1512	966	1302
58 3-HEXANONE	H0318	1149	1084	1434	945	1239
59 CYCLOHEXANONE	C0785	1384	1345	1865	1160	1623
60 2-HEPTANONE	H0184	1293	1225	1612	1061	1411
61 CYCLOHEPTANONE	C0617	1491	1479	1990	1284	1760
62 2-OCTANONE	O0197	1400	1332	1718	1165	1524
63 CYCLOOCTANONE	C0857	1600	1590	2111	1404	1889
64 ACETOPHENONE	A0645	1612	1684	2243	1387	2018
65 2-NONANONE	N0332	1498	1427	1818	1244	1622
66 CYCLONONANONE	C0850	1710	1702	2232	1521	2009
67 2-DECANONE	D0042	1597	1526	1915	1346	1735
68 CYCLODECANONE	C0449	1820	1812	2333	1639	2142
69 CARVONE	C0212	1732	1747	2154	1566	2063
70 2-UNDECANONE	U0039	1696	1619	2012	1469	1810
71 CYCLOUNDECANONE	C06103	1931	1923	2474	1737	2269
72 2-DODECANONE	D0313	1799	1717	2109	1571	1916
73 CYCLODODECANONE	C0609*	2040	2033	2595	1873	2396
74 CYCLOTRIDECANONE	C0924*	2151	2143	2716	1994	2322
75 CYCLOTETRADECANONE	C0930*	2261	2236	2837	2111	2449
ETHERS						
76 ETHYL ETHER	E0477	658	627	758	574	768
77 BUTYL ETHER	E0471	904	974	1099	936	1034
78 FURAN	F0193	693	803	1040	428	964
79 1,4-DIOXANE	D0198	1106	1100	1528	924	1347
80 2-ACETYL,3-METHYL FURAN	F01941	1379	1610	2166	1303	1891
81 2-ACETYL,5-METHYL FURAN	F01942	1612	1641	2211	1319	1931
82 2-PROPIONYL,5-METHYL FURAN	F01943	1479	1366	1987	1300	1801
83 2,4,5-TRIMETHYL OXAZOLE	[illegible]	[illegible]	[illegible]	1393	1045	1443
84 ANISOLE	[illegible]	1251	1133	1783	1139	[illegible]
85 [illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Table 2 *(Continued)*

Substances	Handbook	Zonyl	C.wax 1540	TCEP	Polyph. ether	DEGS
NITROGEN COMPOUNDS						
87 1-NITROMETHANE	M0284	1010	1169	1639	784	1402
88 1-NITROETHANE	E0255	1101	1184	1663	875	1423
89 1-NITROPROPANE	P1210	1184	1248	1722	964	1493
90 2-METHYL,2-NITROPROPANE	P1201e	1201	1138	1579	933	1356
91 3-NITROTOLUENE	T0355	1743	1826	2384	1521	2206
92 ACETONITRILE	A0241	962	1048	1508	701	1262
93 BUTYRONITRILE	B2680	1132	1144	1609	880	1352
94 VALERONITRILE	P0229	1251	1234	1695	987	1481
95 BENZONITRILE	B1291	1530	1643	2172	1298	1942
96 TRIMETHYLAMINE	A0939	700	584	973	476	1036
97 ALLYLAMINE	P1714	784	877	1227	674	1327
98 2-AMINOBUTANE	B2489	828	879	1200	698	1318
99 PYRROLE	P2126	1123	1516	1961	1001	1762
100 PYRIDINE	P1939	1155	1242	1668	994	1507
101 2,3,6-TRIMETHYL PYRIDINE	P2032	1343	1425	1811	1232	1683
102 TRIMETHYL PYRAZINE	P19043	1383	1449	1854	1255	1705
103 2-METHYL,3-ETHYL PYRAZINE	P19042	1354	1438	1825	1236	1685
104 2-METHOXY,3-ISOBUTYL PYRAZINE	P19041	1421	1550	1821	1358	1727
CARBOXYLIC ACIDS						
105 ACETIC ACID	A0058	1035	1425	1823	734	1680
106 PROPIONIC ACID	P1302	1150	1544	1914	884	1764
107 BUTYRIC ACID	B2651	1235	1618	1994	985	1848
108 ISOBUTYRIC ACID	P1518	1204	1572	1908	945	1773
109 3-BUTENOIC ACID	B3016	1248	1738	2140	983	1991
110 A-METHYLBUTYRIC ACID	B2797	1345	1674	2012	1094	1891
111 VALERIC ACID	P0214	1371	1749	2099	1108	1954
112 ISO-VALERIC ACID	B2802	1302	1664	2016	1042	1877
113 HEXANOIC ACID	H0427	1483	1858	2191	1233	1963
114 ISOHEXANOIC ACID	P0291	1417	1779	2128	1148	1877
115 HEPTANOIC ACID	H0144	1595	1966	2283	1358	2039
116 OCTANOIC ACID	O0161	1707	2074	2375	1483	2147
117 NONANOIC ACID	N0534	1819	2182	2467	1608	2236
118 DECANOIC ACID	D0042	1931	2290	2559	1733	2333
119 UNDECANOIC ACID	U0022	2043	2398	2651	1858	2426
120 DODECANOIC ACID	D0295	2155	2506	2744	1982	2519
ESTERS						
121 METHYL ACETATE	A0221	884	840	1164	666	1026
122 ETHYL ACETATE	A0199	960	913	1221	731	1078
123 METHYL PROPIONATE	P1324	955	929	1241	770	1099
124 PROPYL FORMATE	F0144	950	932	1260	762	1112
125 PROPYL ACETATE	A0259	1054	984	1298	844	1152
126 BUTYL ACETATE	A0178	1170	1110	1422	958	1271
127 PROPYL BUTYRATE	B2686	1218	1143	1446	1024	1297
128 AMYL ACETATE	A0253	1269	1209	1513	1058	1349
129 ISOAMYL ACETATE	A0223	1231	1147	1446	1010	1304
130 ISOBUTYL ISOBUTYRATE	P1530	1226	1119	1371	1012	1238
131 METHYL SALICYLATE	B1671	1237	1497	1807	1069	1760
132 ISOAMYL ISOVALERATE	B2807e	1432	1325	1592	1217	1464
133 BENZYL ACETATE	A0173	1651	1749	2344	1378	2082
134 METHYL BENZOATE	B1286	1594	1924	2502	1442	2290
135 2-ETHOXY ETHYL ACETATE	A0446	1358	1333	1776	1112	1573
HALOGEN COMPOUNDS						
136 1-FLUOROOCTANE	O0129	1090	1050	1237	972	1139
137 1,1DIFLUOROTETRACHLOROETHANE	E0223	890	889	1015	784	976
138 1,2DIFLUOROTETRACHLOROETHANE	E0224	899	898	1029	790	991
139 CHLOROFORM	M0306	773	1029	1240	775	1157
140 CARBON TETRACHLORIDE	M0296	788	907	1047	796	1015
141 ETHYLENE CHLORIDE	E0216	863	1081	1398	834	1255
142 TRICHLOROETHYLENE	E0425	862	1025	1210	859	1134
143 1,1,2,2-TETRACHLOROETHANE	E0267	1151	1495	1859	1160	1741
144 HEXACHLOROBUTADIENE	B2453	1363	1522	1735	1376	1713
145 A-CHLOROTOLUENE	T0391	1333	1542	1978	1273	1807
146 1-CHLOROHEXANE	H0330	1008	1065	1266	968	1171
147 1,2-DICHLOROBENZENE	B0335	1317	1523	1862	1279	1749
148 CIS-2-CHLOROISOPROPYL ETHER	E0498	1367	1512	1941	1273	1764
149 2-CHLOROPHENOL	P0613	1367	1835	2274	1270	2120
150 ETHYL BROMIDE	E0195	677	793	1012	663	914
151 1-BROMOPENTANE	P0090	934	1081	1300	973	1199
152 2-BROMOOCTANE	O0117	1242	1329	1523	1214	1418
153 METHYL IODIDE	M0282	643	844	1056	698	967
154 1-IODOBUTANE	B2368	934	1111	1340	989	1234
155 2-IODOBUTANE	B2369	926	1054	1275	946	1178
SULFUR COMPOUNDS						
156 1-ETHANETHIOL	E0328	625	733	970	635	804
157 1,2-ETHANEDITHIOL	E0312	1044	1361	1771	1099	1585
158 1-PROPANETHIOL	P1293	730	863	1079	745	979
159 2-PROPANETHIOL	P1294	693	788	975	677	882
160 ALLYL MERCAPTAN	P1759	740	909	1166	757	1053
161 1-BUTANETHIOL	B2643	849	965	1193	856	1084
162 ISOBUTANETHIOL	P1295	817	920	1123	812	1020
163 TER-BUTANETHIOL	P1296	717	788	957	693	878
164 TETRAHYDROTHIOPHENE	T0224	1038	1179	1509	1035	1363

Table 2 (Continued)

Substances	Handbook	Zonyl	C.wax 1540	TCEP	Polyph. ether	DEGS
165 THIOPHENE	T0187	881	1036	1353	871	1236
166 1-PENTANETHIOL	P0209	951	1073	1293	956	1193
167 ISOPENTANETHIOL	B2648	817	069	1018	805	983
168 DITHIAPENTANE	P0138*	1132	1367	1739	1144	1574
169 2-METHYL THIOPHENE	T0215	996	1154	1441	970	1314
170 HEXANETHIOL	H0420	1062	1189	1407	1070	1297
171 2,5-DIMETHYL THIOPHENE	T0200	1094	1224	1508	1052	1377
172 BENZENETHIOL	B0834	1374	1632	2103	1365	1918
173 1-HEPTANETHIOL	H0142	1164	1282	1508	1166	1407
174 BENZYL MERCAPTAN	T0343	1379	1658	2112	1372	1920
175 1-OCTANETHIOL	O0158	1269	1386	1615	1271	1514
176 1-NONANETHIOL	N0333*	1374	1490	1722	1377	1621
177 1-DECANETHIOL	D0041	1479	1594	1829	1482	1728
178 METHYL SULFIDE	S0313	694	776	1015	654	912
179 ETHYL SULFIDE	S0303	864	930	1171	831	1057
180 PROPYL SULFIDE	S0332	1049	1112	1339	1021	1228
181 PROPYLENE SULFIDE	S0350*	821	965	1238	818	1110
182 ALLYL SULFIDE	S0292	1063	1188	1483	1034	1335
183 ISOAMYL SULFIDE	S0298	1374	1387	1596	1303	1469
184 DIMETHYL DISULFIDE	D0242	935	1138	1425	947	1286
185 DIETHYL DISULFIDE	D0238	1113	1292	1563	1112	1425
186 DIBUTYL SULFIDE	S0295	1255	1322	1525	1217	1400
187 METHYL ETHYL SULFIDE	S0341	626	664	799	611	805
188 METHYL PROPYL SULFIDE	S0348	885	961	1196	853	1076
189 METHYL TRISULFIDE	T0744*	1165	1456	1779	1230	1646
190 METHYL THIOCYANATE	T0175	1160	1325	1821	985	1583
191 METHANETHIOL ACETATE	M03451	1029	1095	1438	899	1286
192 ETHYL ISOTHIOCYANATE	I0228	1077	1265	1651	1019	1461
193 METHANETHIOL PROPANOATE	M03454	1109	1179	1507	995	1357
194 ALLYL ISOTHIOCYANATE	I0216	1144	1383	1765	1101	1591
195 METHANETHIOL BUTYRATE	M03452	1188	1255	1580	1079	1428
196 METHANETHIOL ISOVALERATE	M03453	1239	1284	1586	1117	1444
197 PHENYL ISOTHIOCYANATE	I0236	1486	1731	2104	1437	1985
HYDROCARBONS						
198 ETHYLENE	E0401	222	308	363	270	465
199 PROPYLENE	P1713	324	395	450	360	533
200 1-BUTENE	B2940	422	483	536	450	601
201 PENTENE	P0375	522	581	632	532	689
202 1-HEXENE	H03461	598	634	679	614	712
203 1-HEPTENE	H0197	722	744	794	723	805
204 1-OCTENE	O0208	822	843	890	819	893
205 2-OCTENE(CIS)	O0209	848	879	939	849	931
206 2-ETHYL HEXENE	H0564	837	854	922	824	894
207 2-BUTYNE	B3071	595	790	890	587	838
208 1-OCTYNE	O0221	937	1030	1187	907	1118
209 2-OCTYNE	O0222	973	1075	1229	979	1167
210 BENZENE	B0202	871	979	1257	833	1141
211 TOLUENE	T0275	994	1078	1363	938	1242
212 ETHYL BENZENE	B0758	1084	1162	1439	1035	1333
213 STYRENE	S0159	1150	1280	1620	1094	1510
214 ETHYNYL BENZENE	B0778	1146	1386	1698	1096	1567
215 O-XYLENE	B0660	1112	1182	1475	1044	1360
216 M-XYLENE	B0661	1115	1188	1479	1050	1362
217 P-XYLENE	B0662	1113	1180	1473	1041	1350
218 MESITYLENE	B0975	1233	1311	1587	1155	1481
219 A-PINENE	P0923	1007	1064	1143	1015	1131
lethane						
220 ETHANE	E0162	200	200	200	200	200
221 PROPANE	P1107	300	300	300	300	300
222 BUTANE	B2485	400	400	400	400	400
223 ISOBUTANE	P1200*	376	364	359	358	359
224 PENTANE	P0084	500	500	500	500	500
225 HEXANE	H0319	600	600	600	600	600
226 CYCLOHEXANE	C0637	675	734	816	735	821
227 HEPTANE	H0093	700	700	700	700	700
228 2-METHYL HEPTANE	H0126	780	761	769	760	765
229 3-METHYL HEPTANE	H0127	793	778	789	774	784
230 2,4-DIMETHYL PENTANE	P0133	616	594	544	608	664
231 1-OCTANE	O3112	800	800	800	800	800
232 1-NONANE	N0519	900	900	900	900	900
233 2,2,5-TRIMETHYL HEXANE	H0378	813	757	739	739	757
234 DECANE	D0020	1000	1000	1000	1000	1000
235 DECALIN	D0006	1186	1284	1408	1241	1376
236 HYDRINDANE	H0713	1037	1136	1275	1117	1239
237 UNDECANE	H0019	1100	1100	1100	1100	1100
238 DODECANE	D0284	1200	1200	1200	1200	1200
239 TRIDECANE	T0716	1300	1300	1300	1300	1300
240 TETRADECANE	T0077	1400	1400	1400	1400	1400

[illegible]	[illegible]	[illegible]	[illegible]							
[illegible] ethanol	0.000	0.221	2.35[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
3354 1-propanol	0.000	0.234	2.3[illegible]	[illegible]	0.40[illegible]	[illegible]	0.45[illegible]	0.4[illegible]	[illegible]	0.590
[illegible] 2-propanol	0.000	0.230	2.756	[illegible]	[illegible]	[illegible]	0.51[illegible]	[illegible]	1.821	0.590
[illegible] CH2=CH.CH2OH	0.000	0.250	2.560	1.788	0.450	0.33	0.45	[illegible]	1.996	0.547
3356 1-butanol	0.000	0.242	2.756	1.76[illegible]	0.40[illegible]	0.330	0.45[illegible]	0.499	[illegible]	0.731
3358 2-Me-propan-1-ol	0.000	0.240	2.6[illegible]	1.762	0.400	0.330	0.450	0.499	2.399	0.731
3357 2-butanol	0.000	0.241	2.720	1.762	0.400	0.330	0.510	0.5[illegible]	2.328	0.731
3359 t-butanol	0.000	0.236	2.557	1.725	0.400	0.330	0.570	0.497	[illegible]	0.731
[illegible] 1-pentanol	0.000	0.248	2.756	2.153	0.400	0.330	0.450	0.597	[illegible]	0.872
3361 2-Me-butan-1-ol	0.000	0.248	-	2.163	0.400	0.330	0.450	0.597	-	0.872
3362 3-Me-butan-1-ol	0.000	0.245	2.560	2.136	0.400	0.330	0.450	0.597	-	0.872
3363 2-Me-butan-2-ol	0.000	0.245	2.958	2.136	0.400	0.330	0.570	0.597	-	0.872
3440 cyclopentanol	0.000	0.270	2.990	2.000	0.400	0.330	0.510	0.512	-	0.742
3368 1-hexanol	0.000	0.252	2.890	2.553	0.400	0.330	0.450	[illegible]	3.610	1.013
3369 2-hexanol	0.000	0.250	2.990	2.530	0.400	0.330	0.51[illegible]	[illegible]	3.34[illegible]	1.013
3370 3-hexanol	0.000	0.251	-	2.543	0.400	0.330	0.51[illegible]	[illegible]	3.44[illegible]	1.013
3372 2-Me-pentan-2-ol	0.000	0.248	-	2.512	0.400	[illegible]	0.57[illegible]	[illegible]	3.18[illegible]	1.013
3374 3-Me-pentan-3-ol	0.000	0.252	-	2.553	0.400	[illegible]	0.57[illegible]	[illegible]	3.277	1.013
3389 1-heptanol	0.000	0.256	2.924	2.954	0.400	0.330	0.450	0.789	4.115	1.154
3405 1-octanol	0.000	0.258	2.958	3.341	0.400	0.330	0.450	0.880	4.619	1.295
3416 1-nonanol	0.000	0.260	2.958	3.731	0.400	0.330	0.450	[illegible]	5.124	1.435
3426 1-decanol	0.000	0.262	2.592	4.129	0.400	0.330	0.450	1.[illegible]	5.628	1.576
1551 acetaldehyde	0.000	0.205	7.236	0.832	0.670	0.[illegible]	0.420	0.287	1.27[illegible]	0.406
1552 propionaldehyde	0.000	0.223	6.350	1.220	0.650	0.000	0.410	[illegible]	1.815	0.547
1553 butyraldehyde	0.000	0.234	7.398	1.510	0.630	0.000	0.41[illegible]	0.43	2.27[illegible]	0.698
1554 iso-butyraldehyde	0.000	0.228	-	1.569	0.620	[illegible]	0.41[illegible]	[illegible]	-	0.689
1570 trans-MeCH=CHCHO	0.000	0.262	12.530	1.590	0.750	[illegible]	[illegible]	0.44[illegible]	-	0.645
1555 pentanal	0.000	0.239	6.760	1.981	0.63[illegible]	[illegible]	0.41	[illegible]	2.770	0.829
1590 benzaldehyde	1.000	0.317	7.563	2.767	0.92[illegible]	[illegible]	0.44[illegible]	[illegible]	3.985	0.873
1651 2-propanone	0.000	0.220	8.294	1.207	0.710	0.000	0.49[illegible]	0.380	1.760	0.547
1652 2-butanone	0.000	0.231	7.618	1.539	0.670	0.000	0.480	0.477	2.287	0.698
1657 2-pentanone	0.000	0.237	7.290	1.965	0.670	0.000	0.48[illegible]	0.574	2.755	0.829
1706 cyclopentanone	0.000	0.262	10.390	1.586	0.76[illegible]	[illegible]	0.52[illegible]	0.512	[illegible]	0.720
1659 2-hexanone	0.000	0.243	7.0[illegible]	2.357	0.65	0.000	0.480	0.67[illegible]	3.262	0.970
1660 3-hexanone	0.000	0.243	7.023[e]	2.357	0.65[illegible]	0.000	0.450	0.668	3.310	0.970
1708 cyclohexanone	0.000	0.269	9.000	2.316	0.750	0.000	0.500	0.571	3.616	0.861
1664 2-heptanone	0.000	0.247	6.810	2.744	0.630	0.000	0.480	0.76[illegible]	3.760	1.111
1675 2-octanone	0.000	0.250	7.400	3.128	0.610	0.000	0.480	0.86[illegible]	4.257	1.251
1750 acetophenone	1.000	0.312	9.000	3.164	0.900	0.000	0.490	0.69[illegible]	4.483	1.014
1685 2-nonanone	0.000	0.254	7.300	3.536	0.610	0.000	0.480	0.956	4.755	1.392
1690 2-decanone	0.000	0.256	7.200[e]	3.924	0.610	0.000	0.480	1.051	5.260	1.533
1352 Et2O	0.000	0.217	1.220	1.586	0.270	0.000	0.470	0.505	2.061	0.731
1355 n-Bu2O	0.000	0.242	1.369	3.134	0.240	0.000	0.460	0.897	4.001	1.295
1414 furan	1.000	0.254	0.436	1.361	-	0.000	-	0.[illegible]	-	0.536
1421 dioxan	0.000	0.254	0.000	1.730	0.550	0.000	0.740	0.491	2.797	0.681
1450 PhOMe	1.000	0.303	1.904	2.775	0.730	0.000	0.320	0.630	3.926	0.916
1550 methyl acetate	0.000	0.220	2.955	1.333	0.600	0.000	0.420	0.424	1.960	0.606
1551 ethyl acetate	0.000	0.227	3.168	1.696	0.550	0.000	0.450	0.521	2.376	0.747
1581 methyl propionate	0.000	0.230	2.890	1.718	0.500	[illegible]	0.4[illegible]	0.524	2.459	0.747
1562 n-propyl acetate	0.000	0.234	3.420	2.078	0.520	0.000	0.450	0.622	2.878	0.888
1564 n-butyl acetate	0.000	0.239	3.240	2.457	0.500	0.000	0.450	0.716	3.379	1.028
1567 pentyl acetate	0.000	0.244	3.067	2.852	0.450	0.000	0.450	0.721	3.881	1.169
1873 benzyl acetate	1.000	0.306	3.240	3.715	0.530	0.000	0.540	0.874	-	1.214
1921 methyl benzoate	1.000	0.302	3.240	3.240	0.770	0.000	0.[illegible]	[illegible]	4.534	1.073
1950 MeCOOH	0.000	0.227	3.028	1.036	0.450	0.710	0.54	[illegible]	[illegible]	0.465
1951 EtCOOH	0.000	0.235	3.067	-	0.450	0.6[illegible]	0.54[illegible]	0.41[illegible]		0.606
1954 n-PrCOOH	0.000	0.241	1.510	-	0.450	0.6[illegible]	0.540	0.51[illegible]	-	0.747
1955 iPrCOOH	0.000	0.239	1.190	-	0.45	0.600	0.54	0.51[illegible]	-	0.747
1956 n-BuCOOH	0.000	0.247	1.590	-	0.450	0.600	0.540	0.6[illegible]	-	0.888
1957 i-BuCOOH	0.000	0.244	1.740	-	0.500	0.600	0.54	0.518	-	0.888
1958 n-pentCOOH	0.000	0.251	1.280	-	0.500	0.600	0.540	0.708		1.029
1964 n-hexCOOH	0.000	0.251	1.30[e]	-	0.450	0.600	0.540	0.80[illegible]		1.169
1969 n-heptCOOH	0.000	0.258	1.3[illegible]	-	0.480	0.6[illegible]	[illegible]	[illegible]		1.310
1979 n-octCOOH	0.000	0.259	1.30[e]		0.450	[illegible]	[illegible]	[illegible]	-	1.592
[illegible]	0.500	0.267	1.320	1.847	0.580	[illegible]	0.[illegible]	[illegible]	2.48[illegible]	0.617
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]				[illegible]	[illegible]	[illegible]

[illegible]	1122-tetraCl-ethane	0.500	[illegible]	1.742	2.551	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
[illegible]	4-chlorotoluene	1.000	0.302	4.380	2.960	0.57	[illegible]	[illegible]	[illegible]		[illegible]
1002	o-dichlorobenzene	1.000	0.319	6.250	[illegible]	0.800	0.000	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]-C6H4OH	1.000	0.320	4.796	2.374	-	-		[illegible]	[illegible]	0.898
605	EtBr	0.000	0.255	4.121	1.441	0.430	0.000	[illegible]	[illegible]	[illegible]	0.565
624	1-bromopentane	0.000	0.266	4.840	1.878	-	[illegible]	[illegible]	[illegible]	-	0.706
651	MeI	0.000	0.313	2.624	1.590	0.400	[illegible]	0.070	0.344	[illegible]	0.508
670	n-BuI	0.000	0.294	4.494	2.734	0.500	0.000	0.067	[illegible]	-	0.930
2101	MeNO2	0.000	0.233	11.972	0.988	0.850	0.000	0.250	0.343	1.892	0.424
2102	EtNO2	0.000	0.238	13.320	1.345	0.820	0.000	0.250	0.445	2.367	0.565
2103	n-PrNO2	0.000	0.243	13.396	1.716	0.790	0.000	0.250	0.540	2.710	0.706
2201	MeCN	0.000	0.212	15.366	0.856	0.750	0.000	0.370	0.271	1.560	0.404
2203	n-PrCN	0.000	0.224	15.560	1.605	0.680	0.000	0.370	0.465	-	0.686
2205	n-BuCN	0.000	0.241	16.970	1.993	-	0.000	0.370	[illegible]	-	0.827
2241	PhCN	1.000	0.308	17.470	2.633	0.900	0.000	0.360	0.590	4.004	0.871
2341	[illegible]	0.000	0.222	0.375	1.401	0.140	0.000	0.650	[illegible]	1.620	0.631
2351	pyrrole	1.000	0.298	3.335	1.719	-		-	[illegible]	2.865	0.577
2701	pyridine	1.000	0.299	4.796	2.013	0.870	0.000	0.640	[illegible]	[illegible]	0.675
3552	EtSH	0.000	0.259	2.460	1.435	0.350	0.100	0.220	[illegible]	2.173	0.554
3553	nPrSH	0.000	0.263	2.280	1.823	0.35	0.100	0.20	0.430	2.685	0.695
3554	iPrSH	0.000	0.256	2.560	1.779	0.35	0.100	0.20	0.480	2.406	0.695
3555	n-BuSH	0.000	0.256	[illegible]	2.224	0.350	0.100	0.180	[illegible]	3.242	0.836
3558	tBuSH	0.000	0.254	-	2.123	-	0.100	-	0.575	2.558	0.836
3601	thiophene	1.000	0.308	0.325	1.974	-	-	-	0.443	2.943	0.641
3602	2-Me-thiophen	1.000	0.304	0.449	2.377	-	-	-	0.539	-	0.762
3603	25-diMe-thiophen	1.000	0.301	0.260	2.778	-	-	-	0.635	-	0.923
3565	PhSH	1.000	0.337	1.440	2.966	-	-	-	0.600	-	0.880
3579	Me2S	0.000	0.266	2.250	1.474	0.360	0.000	0.250	0.376	2.238	0.554
3580	Et2S	0.000	0.265	2.310	2.215	0.360	0.000	0.280	0.576	3.104	0.836
3581	nPr2S	0.000	0.268	2.430	2.996	0.36	0.000	0.28	0.768	-	1.118
[illegible]	Me2S2	0.000	0.308	3.880	2.208	0.300	0.000	[illegible]	[illegible]	3.549	0.717
370	ethene	0.000	0.222	0.000	0.770	0.090	0.000	[illegible]	[illegible]	1.289	0.347
371	propene	0.000	0.219	0.134	1.069	0.090	0.000	[illegible]	0.336	1.946	0.488
373	1-butene	0.000	0.240	0.116	1.510	0.080	0.000	0.080	0.427	1.491	0.629
380	1-pentene	0.000	0.227	0.115	1.748	0.080	0.000	0.070	0.531	2.013	0.770
392	1-hexene	0.000	0.234	0.116	2.132	0.080	0.000	0.070	0.618	2.547	0.911
406	1-heptene	0.000	0.242	0.116	2.546	0.080	0.000	0.070	0.715	3.063	1.052
419	1-octene	0.000	0.247	0.116	2.944	0.080	0.000	0.070	0.812	3.591	1.192
453	2-butyne	0.000	0.238	0.656	1.395	0.200	0.000	0.170	0.405	-	0.586
468	3-octyne	0.000	0.251	0.656	2.886	0.200	0.100	0.170	[illegible]	-	1.150
469	2-octyne	0.000	0.257	0.656	2.956	0.200	0.000	0.170	[illegible]	-	1.150
751	benzene	1.000	0.295	0.000	2.112	0.590	0.000	0.100	0.491	2.803	0.716
752	toluene	1.000	0.292	0.130	2.502	0.540	0.000	0.110	[illegible]	3.344	0.857
766	PhEt	1.000	0.292	0.348	2.914	0.480	0.000	0.120	[illegible]	3.765	0.998
343	styrene	1.000	0.317	0.000	3.027	-	0.000	-	0.659	3.908	0.955
795	PhOMe	1.000	0.300	0.533	2.736	-	-	-	0.628	-	0.912
753	o-xylene	1.000	0.297	0.384	2.964	0.470	0.000	0.120	0.683	3.937	0.998
754	m-xylene	1.000	0.293	0.160	2.924	0.470	0.000	0.120	[illegible]	3.864	0.998
755	p-xylene	1.000	0.292	0.000	2.914	0.430	0.000	0.12	[illegible]	3.858	0.998
758	mesitylene	1.000	0.294	0.000	3.349	0.410	0.000	[illegible]	[illegible]	4.399	1.139
51	ethane	0.000	0.025	0.000	- ?	0.000	0.000	0.000	0.262	0.492	0.390
52	propane	0.000	0.181	0.000	0.961	0.000	0.000	0.000	0.360	1.050	0.531
53	n-butane	0.000	0.205	0.000	1.378	0.000	0.000	0.000	0.455	1.615	0.672
54	iso-butane	0.000	0.197	0.000	1.324	0.000	0.000	0.000	0.458	1.409	0.672
55	n-pentane	0.000	0.219	0.000	1.780	0.000	0.000	[illegible]	[illegible]	[illegible]	0.813
56	n-hexane	0.000	0.229	0.000	2.195	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.954
287	cyclohexane	0.000	0.257	0.372	[illegible]	0.000	0.000	0.000	[illegible]	[illegible]	0.845
62	n-heptane	0.000	0.236	0.000	2.594	0.000	[illegible]	[illegible]	[illegible]	[illegible]	1.095
73	2-Me-heptane	0.000	0.240	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-	1.236
74	3-methylheptane	0.000	0.242	0.000	[illegible]	0.00	0.000	0.000	[illegible]		1.236
69	24-diMe-pentane	0.000	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.095
[illegible]	n-octane	0.000	0.241	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	n-nonane	0.000	0.245	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.377
[illegible]	225-trimethylhexane	0.000	0.242	[illegible]	[illegible]	0.00	0.000	0.000	[illegible]		1.377
[illegible]	n-decane	0.000	0.249	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.518
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.658
											[illegible]

	δ	$H(n^2)$	μ	$(n^2)/V_x$	π_2^*	α_2	β_2	V_I	$Log L$	V_x
174 n-tridecane	0.[illegible]	0.256	0.[illegible]	[illegible]	0.00[illegible]	[illegible]	0.0[illegible]	1.[illegible]	6.[illegible]	1.9[illegible]
[illegible] n-tetradecane	[illegible]	[illegible]	[illegible]	5.26[illegible]	0.[illegible]	[illegible]	[illegible]	1.[illegible]	[illegible]	[illegible]

Table 4. Values of b used in equation (8) and (9).

Stationary phase	b
Zonyl	0.203
CWAX 1540	0.214
TCEP	0.178
Polyph ether	0.262
DEGS	0.190

Table 5 PARAMETER COEFFICIENTS OBTAINED FROM REGRESSIONS USING V_x

									CORRELATION %					
ZONYL E7														
d	π_2^*	α_m	β_m	V_x	C	n	r	s.d.	d	π_2^*	α_m	β_m	V_x	C
0.144	1.781	0.602	0.354	1.511	-2.313	104	0.9799	0.133	99.7	100	99.9	99.8	100	100
$f(n^2)$	μ^2	α_m	β_m	V_x	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	V_x	C
9.266	0.063	0.281	1.205	1.158	-4.0	100	0.9579	0.187	100	100	92.4	100	100	100
CARBOWAX														
d	π_2^*	α_m	β_m	V_x	C	n	r	s.d.	d	π_2^*	α_m	β_m	V_x	C
0.236	2.17	2.343	-0.443	1.446	-2.206	103	0.9714	0.172	99.9	100	100	99.7	100	100
$f(n^2)$	μ^2	α_m	β_m	V_x	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	V_x	C
13.051	0.068	1.809	0.842	0.968	-4.648	98	0.9548	0.215	100	100	100	100	100	100
TRICYANOETHOXYPROPANE														
d	π_2^*	α_m	β_m	V_x	C	n	r	s.d.	d	π_2^*	α_m	β_m	V_x	C
0.231	2.552	1.873	0.065	1.189	-1.787	108	0.9639	0.213	99.6	100	100	30.4	100	100
$f(n^2)$	μ^2	α_m	β_m	V_x	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	V_x	C
13.92	0.088	1.445	1.388	0.651	-4.368	98	0.9494	0.248	100	100	100	100	100	100

Table 5. CONT.

									CORRELATION %					
POLYPHENYL ETHER														
δ	π_2^*	α_m	β_m	V_x	C	n	r	s.d.	δ	π_2^*	α_m	β_m	V_x	C
0.360	1.725	0.833	-0.278	1.847	-2.765	105	0.9768	0.158	100	100	100	97.3	100	100
$f(n^2)$	μ^2	α_m	β_m	V_x	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	V_x	C
12.534	0.05	0.474	0.704	1.352	-5.114	96	0.9744	0.160	100	100	99.9	100	100	100
DIETHYLENE GLYCOL SUCCINATE														
δ	π_2^*	α_m	β_m	V_x	C	n	r	s.d	δ	π_2^*	α_r	β_m	V_x	C
0.269	2.341	2.049	-0.274	1.251	-1.857	106	0.9621	0.199	99.9	100	100	88.6	100	100
$f(n^2)$	μ^2	α_m	β_m	V_x	C	n	r	s.d	$f(n^2)$	μ^2	α_m	β_m	V_x	C
14.047	0.069	1.411	1.210	0.727	-4.503	99	0.9473	0.236	100	100	100	100	100	100

Table 6. Parameter Coefficients obtained from regressions using Log L16									CORRELATION %					
ZONYL E7														
δ	π_2^*	α_m	β_m	Log L16	C	n	r	s.d.	δ	π_2^*	α_m	β_m	Log L16	C
-0.038	1.029	-0.065	0.708	0.422	-1.978	90	0.9910	0.09	68.6	100	58.9	100	100	100
$f(n^2)$	μ^2	α_m	β_m	Log L16	C	n	r	s.d	$f(n^2)$	μ^2	α_m	β_m	Log L16	C
3.389	0.052	-0.094	1.126	0.395	-2.611	87	0.9826	0.124	100	100	60.9	100	100	100
CARBOWAX														
δ	π_2^*	α_m	β_m	Log L16	C	n	r	s.d.	δ	π_2^*	α_m	β_m	Log L16	C
0.034	1.549	1.743	-0.141	0.416	-1.93	94	0.9847	0.128	50.7	100	100	82.1	100	100
$f(n^2)$	μ^2	α_m	β_m	Log L16	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	Log L16	C
7.559	0.065	1.514	0.67	0.339	-3.376	88	0.9735	0.166	100	100	100	100	100	100
TRICYANOETHOXYPROPANE														
δ	π_2^*	α_m	β_m	Log L16	C	n	r	s.d.	δ	π_2^*	α_m	β_m	Log L16	C
0.012	2.178	1.572	0.112	0.355	-1.63	94	0.9838	0.149	16.3	100	100	60	100	100
$f(n^2)$	μ^2	α_m	β_m	Log L16	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	Log L16	C
10.903	0.086	1.247	1.402	0.25	-3.749	89	0.9566	0.246	100	100	100	100	100	100

Table 6 CONT.

POLYPHENYL ETHER									CORRELATION %					
δ	π_2^*	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	π_2^*	α_m	β_m	$\log L^{16}$	C
0.043	0.998	0.439	0.036	0.523	-2.412	94	0.9943	0.084	86.9	100	100	40.3	100	100
$f(n^2)$	μ^2	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	$\log L^{16}$	C
5.433	0.04	0.315	0.525	0.463	-3.444	87	0.9888	0.109	100	100	99.6	100	100	100
DIETHYLENE GLYCOL SUCCINATE														
δ	π_2^*	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	π_2^*	α_m	β_m	$\log L^{16}$	C
0.066	1.843	1.548	-0.041	0.375	-1.69	94	0.9805	0.176	75.3	100	100	24.9	100	100
$f(n^2)$	μ^2	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ^2	α_m	β_m	$\log L^{16}$	C
9.472	0.069	1.256	1.074	0.26	-3.453	88	0.9660	0.190	100	100	100	100	100	100

Table 7.									CORRELATION %					
POLYPHENYLETHER USING δ AND μ^2														
δ	μ^2	α_m	B_m	V_x	C	n	r	s.d.	δ	μ^2	α_m	B_m	V_x	C
0·931	0·066	0·877	0·608	1·724	-2·534	96	0·9507	0·215	100	100	99·9	99·9	100	100
δ	μ^2	α_m	B_m	Log46	C	n	r	s.d.	δ	μ^2	α_m	B_m	Log46	C
0·413	0·051	0·513	0·445	0·509	-2·313	84	0·9922	0·093	100	100	99·9	100	100	100
POLYPHENYLETHER USING MR_x AND μ^2														
MR_x	μ^2	α_m	B_m	V_x	C	n	r	s.d.	MR_x	μ^2	α_m	B_m	V_x	C
1·549	0·048	0·438	0·757	-2·495	-2·047	95	0·9825	0·133	100	100	99·9	100	100	100
MR_x	μ^2	α_m	B_m	Log46	C	n	r	s.d.	MR_x	μ^2	α_m	B_m	Log46	C
-0·727	0·023	0·145	0·312	1·09	-2·22	86	0·9820	0·134	100	99·9	72·7	99·8	100	100

Table 8									CORRELATION %					
TRICYANOETHOXYPROPANE						DOMINANT DIPOLES								
$f(n^2)$	μ^2	α_m	β_m	V_x	C	n	r	S.d.	$f(n^2)$	μ^2	α_m	β_m	V_x	C
14.267	0.086	1.514	1.333	0.709	-4.537	82	0.9620	0.228	100	100	100	100	100	100
$f(n^2)$	μ^2	α_m	β_m	$\text{Log}L^{16}$	C	n	r	S.d	$f(n^2)$	μ^2	α_m	β_m	$\text{Log}L^{16}$	C
10.523	0.082	1.518	1.262	0.251	-3.684	72	0.9736	0.198	100	100	100	100	100	100
TRICYANOETHOXYPROPANE						DOMINANT DIPOLES								
MR_x	μ^2	α_m	β_m	V_x	C	n	r	S.d.	MR_x	μ^2	α_m	β_m	V_x	C
2.049	0.092	1.642	1.224	-4.429	-0.998	81	0.9768	0.167	100	100	100	100	100	100
MR_x	μ^2	α	β	$\text{Log}L^{16}$	C	n	r	S.d.	MR_x	μ^2	α_m	β_m	$\text{Log}L^{16}$	C
-1.402	0.045	0.833	1.081	1.444	-1.259	72	0.9490	0.267	100	100	100	100	100	100

Table 8 CONT. TRICYANOETHOXYPROPANE

									CORRELATION %					
δ	π_2^x	α_m	β_m	V_x	c	n	r	s.d.	δ	π_2^x	α_m	β_m	V_x	c
0.171	2.808	2.105	-0.385	1.243	-1.844	89	0.9731	0.193	100	100	100	90	100	100
δ	π_2^x	α_m	β_m	$\log L^{16}$	c	n	r	s.d.	δ	π_2^x	α_m	β_m	$\log L^{16}$	c
0.08	2.154	1.629	-0.015	0.36	-1.643	78	0.9884	0.134	81.6	100	100	73	100	100
TRICYANOETHOXYPROPANE														
δ	μ^2	α_m	β_m	V_x	c	n	r	s.d.	δ	μ^2	α_m	β_m	V_x	c
1.081	0.096	1.930	1.456	1.117	-1.620	79	0.9587	0.250	100	100	100	100	100	100
δ	μ^2	α_m	β_m	$\log L^{16}$	c	n	r	s.d.	δ	μ^2	α_m	β_m	$\log L^{16}$	c
0.851	0.113	2.02	0.96	0.34	-1.505	71	0.9856	0.149	100	100	100	100	100	100

Table 9.

									CORRELATION %					
ZONYL E7														
$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C
2.528	0.191	-0.293	0.997	0.404	-2.472	85	0.9815	0.128	99.9	100	99.1	100	100	100
CARBOWAX														
$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C
6.933	0.254	1.44	0.30	0.352	-3.302	85	0.9753	0.162	100	100	100	96.2	100	100
TRICYANOETHOXYPROPANE														
$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C
9.300	0.292	0.967	1.194	0.272	-3.482	85	0.9666	0.212	100	100	99.9	100	100	100
POLYPHENYL ETHER														
$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C
5.166	0.172	0.261	0.231	0.470	-3.423	85	0.9896	0.106	100	100	98.5	98.6	100	100
DIETHYLENE GLYCOL SUCCINATE														
$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	$f(n^2)$	μ	α_m	β_m	$\log L^{16}$	C
9.468	0.221	0.995	0.976	0.268	-3.513	85	0.9666	0.191	100	100	100	100	100	100

Table 10.

									CORRELATION %					
ZONYL E7														
δ	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	μ	α_m	β_m	$\log L^{16}$	C
0.345	0.193	-0.188	1.014	0.415	-1.940	85	0.9916	0.091	100	100	97	100	100	100
	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.		μ	α_m	β_m	$\log L^{16}$	C
	0.252	-0.053	0.735	0.415	-1.935	62	0.9951	0.071		100	50.2	100	100	100
CARBOWAX														
δ	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	μ	α_m	β_m	$\log L^{16}$	C
0.552	0.315	1.616	0.075	0.404	-1.851	88	0.9837	0.135	100	100	100	48.8	100	100
	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.		μ	α_m	β_m	$\log L^{16}$	C
	0.369	1.850	-0.115	0.410	-1.902	65	0.9884	0.120		100	100	65.6	100	100
TRICYANOETHOXYPROPANE														
δ	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	μ	α_m	β_m	$\log L^{16}$	C
0.812	0.395	1.262	0.833	0.336	-1.535	83	0.9865	0.136	100	100	100	100	100	100
	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.		μ	α_m	β_m	$\log L^{16}$	C
	0.530	1.810	0.075	0.343	-1.589	63	0.9872	0.138		100	100	34.5	100	100

Table 10 cont.									CORRELATION %					
POLYPHENYL ETHER														
δ	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	μ	α_m	β_m	$\log L^{16}$	C
0.424	0.199	0.410	0.173	0.510	-2.531	87	0.9927	0.093	100	100	99.9	96.3	100	100
	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.		μ	α_m	β_m	$\log L^{16}$	C
	0.232	0.486	0.06	0.519	-2.403	63	0.9950	0.076		100	100	55.3	100	100
DIETHYLENE GLYCOL SUCCINATE														
δ	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.	δ	μ	α_m	β_m	$\log L^{16}$	C
0.691	0.355	1.458	0.314	0.350	-1.559	86	0.9810	0.149	100	100	100	96.7	100	100
	μ	α_m	β_m	$\log L^{16}$	C	n	r	s.d.		μ	α_m	β_m	$\log L^{16}$	C
	0.439	1.761	-0.032	0.366	-1.661	62	0.9846	0.132		100	100	15.6	100	100

Table 11. Further values of log L^{16} obtained at 298.15 K relative to n-octane standard.

Solute	log L^{16}
n-Octane	3.677
Benzonitrile	3.994
Benzaldehyde	3.985
2-Methyl-3-pentanol	3.183
3-Methyl-3-pentanol	3.227
3-Hexanol	3.440
Ethyleneglycol diacetate	4.083
Pyrrole	2.866
2-Chlorophenol	4.937
N-Methylaniline	4.494
2-Chlorotoluene	4.160
Methyl benzoate	4.634
Mesitylene	4.399

DATE
FILMED
5 8